Multiscale Modeling of Corrosion and Oxidation Performance and Their Impact on High-temperature Fatigue of Automotive Exhaust Manifold Components

Project ID: MAT163

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Ford Motor Company

June 4, 2020

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2020 Vehicle Technologies AMR

Overview

Timeline

- Project start date: November 2018
- Project end date: October 2021
- Percent complete: 40%

Budget

- Total project funding:
  - DOE share: $1.26M

    Contractor share: $0.58M

Partners

- The Ohio State University
- Missouri Science and Technology
- Oak Ridge National Laboratory

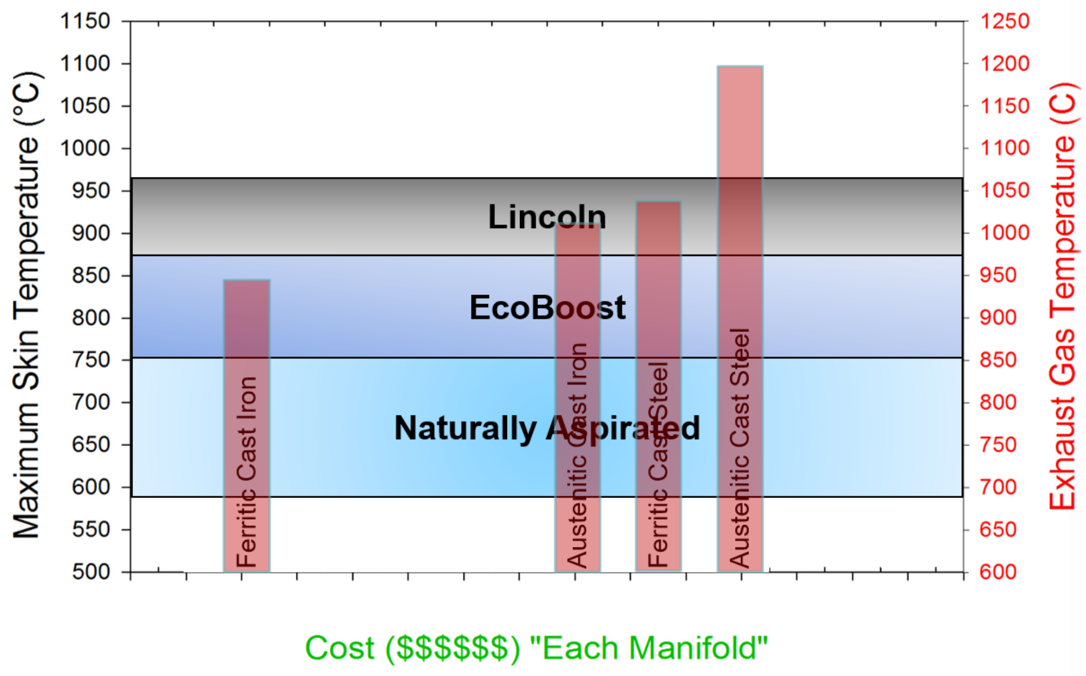
Barriers

- Gaps between micro-scale and meso-scale modeling
- In-site Thermo-Mechanical Fatigue test in exhaust gas environment
- Component level demonstration
- Light-Duty Vehicles Technical Requirements and Gaps for Lightweight and Propulsion Materials Workshop Report, February 2013, Section 4

Relevance

- Impacts:

  The successful development of computation tools to predict corrosion/oxidation performance, and their impact on high-temperature fatigue will enable the acceleration of heat-resist alloys solutions to meet the increased exhaust temperature requirement, which leads to reduce automotive emission



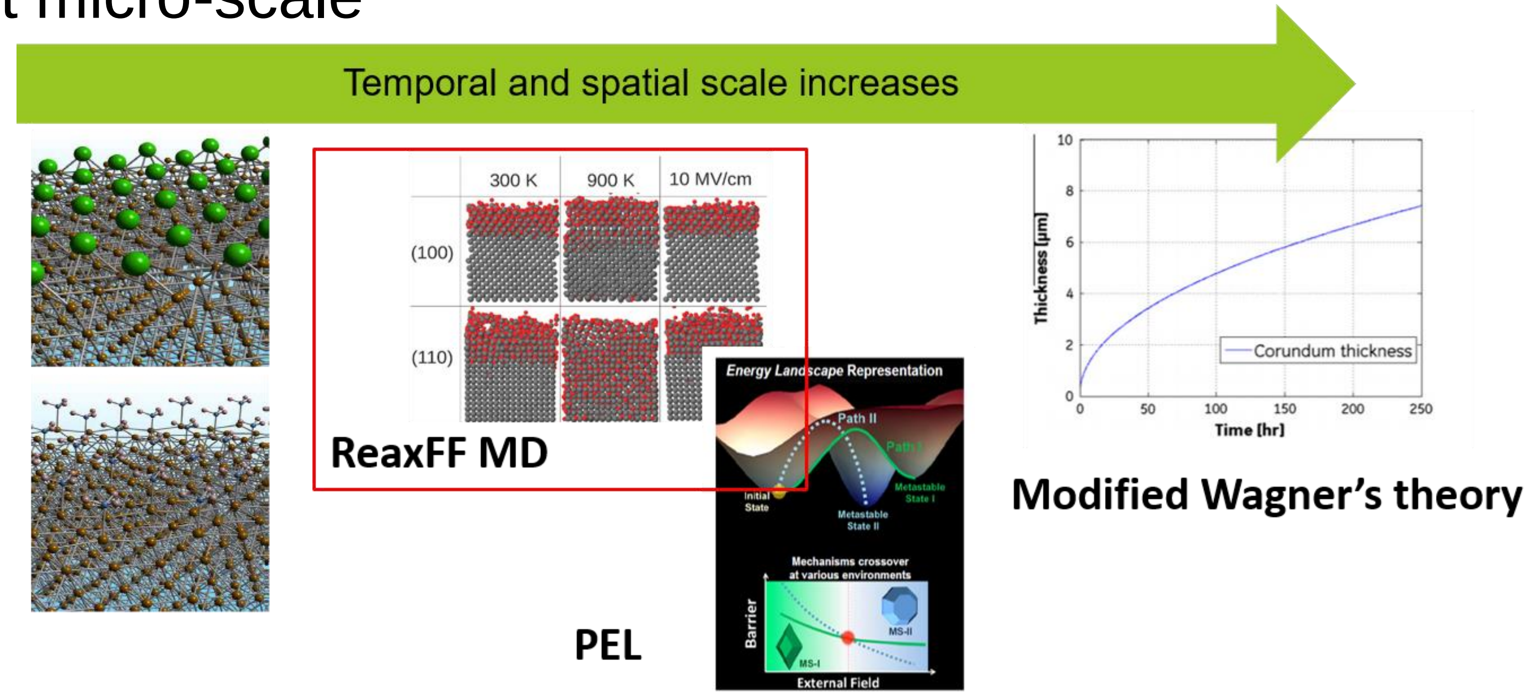
- Overall Objectives:
  - Develop computational tools to predict corrosion/oxidation behavior
  - Conduct statics and cyclic corrosion/oxidation trials and characterize the tests samples
  - Perform TMF tests and develop corrosion/oxidation-fatigue model
  - Demonstrate on components

Milestones

Data	Milestones and Go/No-Go decision	Status
June 2020	Develop the corrosion/oxidation performance model for SiMo-type cast iron alloys (Technical) 1. Complete the development of ReaxFF MD simulation for SiMo-Type alloys; 2. Develop PEL modeling for SiMo-type alloy; 3. Develop more reliable force field for SiMo-Type alloys with exhaust gas species;	70%
March 200	Conduct experiments to validate corrosion/oxidation performance model for SiMo-type cast iron alloys (Technical) 1. Complete static corrosion/oxidation tests for SiMo-type alloys in control and exhaust gas 2. Conduct corrosion/oxidation tests for SiMo-type alloys in control and exhaust gas	80%
September 2020	Develop the corrosion/oxidation-fatigue model for SiMo-type cast iron alloys (Technical) 1. Conduct TMF test for SiMo-type alloys corroded/oxidized in SiMo-type 2. Develop a experiment system for in-site TMF tests in control and exhaust gas	60%
September 2020	Complete corrosion/oxidation performance and corrosion/oxidation-fatigue modeling (Go/No0Go)	On-going

Approach

- Multi-scale modeling of corrosion/oxidation performance
  - Density Function Theory (DFT) calculation to develop robust force field to quantify the interaction between iron alloys and exhaust gas spices
  - Reaction Force Field Molecular Dynamic (ReaxFF MD) to simulate the corrosion/oxidation process at micro-scale
  - Potential Energy Landscape (PEL) to model atomic migration mechanism at larger time scale
  - Modifed Magner’s theory using inputs from low-level simulation to predict the growth kinetics of corrosion/oxidation products

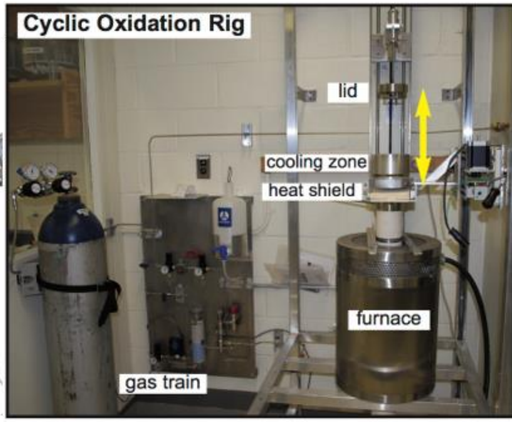


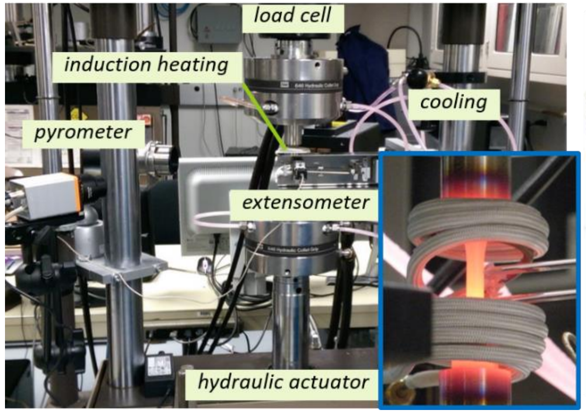
Approach

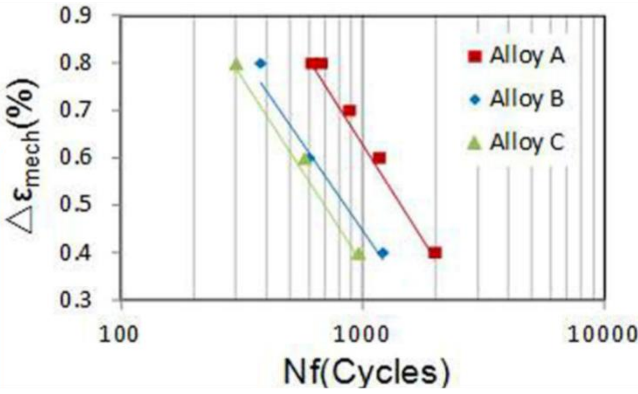
- Static and cyclic corrosion/oxidation tests in control and exhaust gas, with characterization of products, to validate multi-scale simulation

- Ex-site and in-site Thermomechanical fatigue tests and empirical model development for life prediction

2-zone furnace for static oxidation

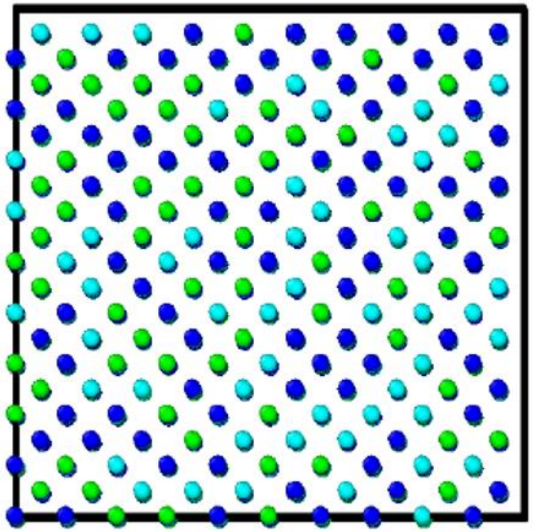






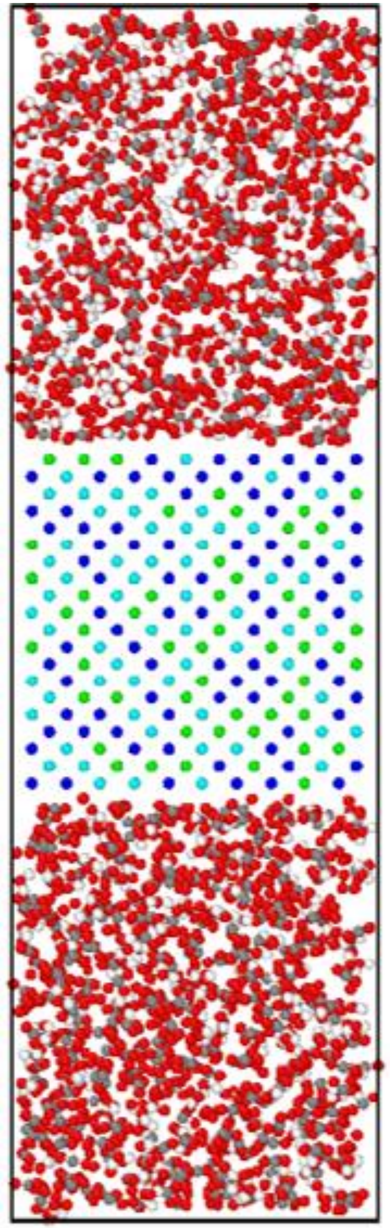
Technical Accomplishment

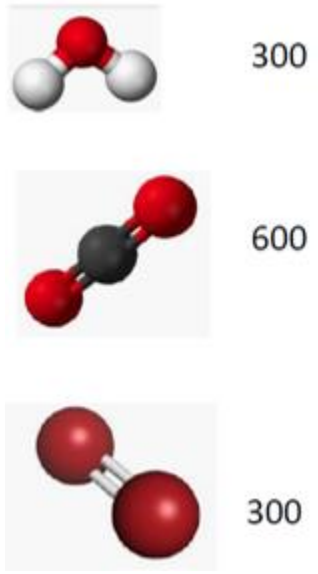
- ReaxFF MD enables the simulation of breaking and forming bonds during chemical reactions
- The reaction of bcc Iron with alloying elements, X and Y, in exhaust gas were studied
- NVT, 30A*30A*100A domain, 5000 times atm to accelerate reaction rates



	1)	2)
Fe	75%	50%
X	20%	25%
Y	5%	25%

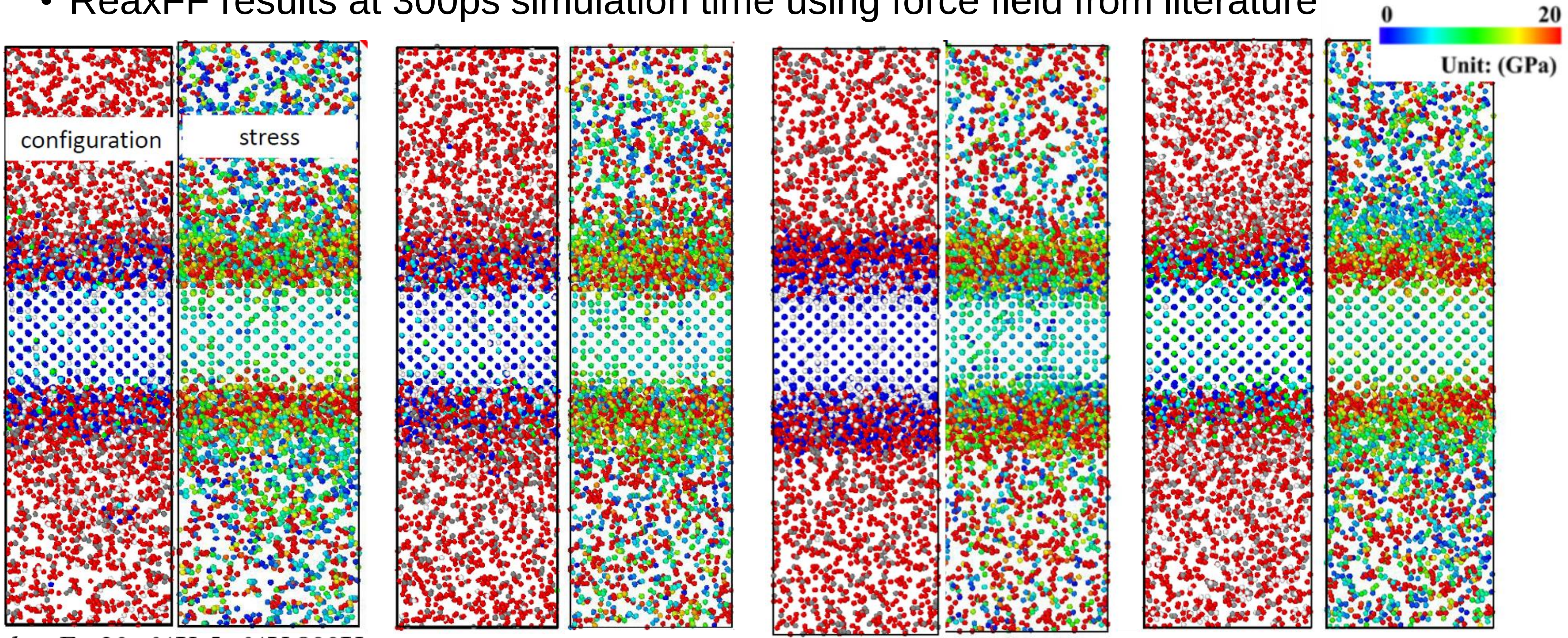
Total Number : 2000





Technical Accomplishment

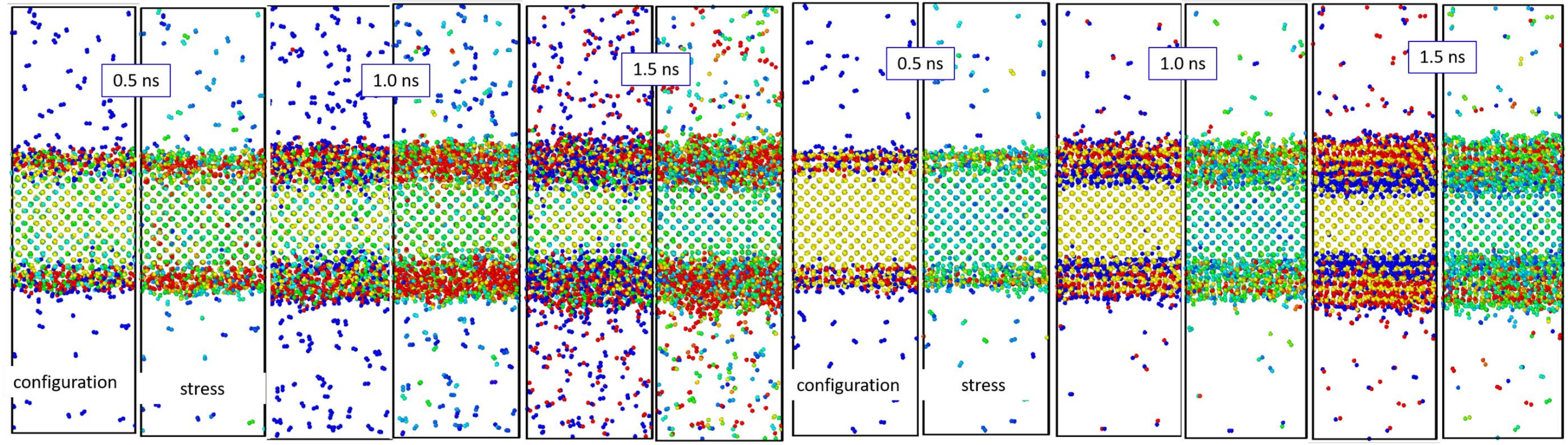
- ReaxFF results at 300ps simulation time using force field from literature



bcc-Fe-20at%X-5at%Y-**800K** *bcc*-Fe-20at%X-5at%Y-**1200K** *bcc*-**pure_Fe**-1200K *bcc*-**Fe-25at%X-25at%Y**-1200K

Technical Accomplishment

- Modification: (1)New force field was employed to increase stability of oxidation products and (2)More realistic gas pressure ~1atm, with only oxygen and water vapor



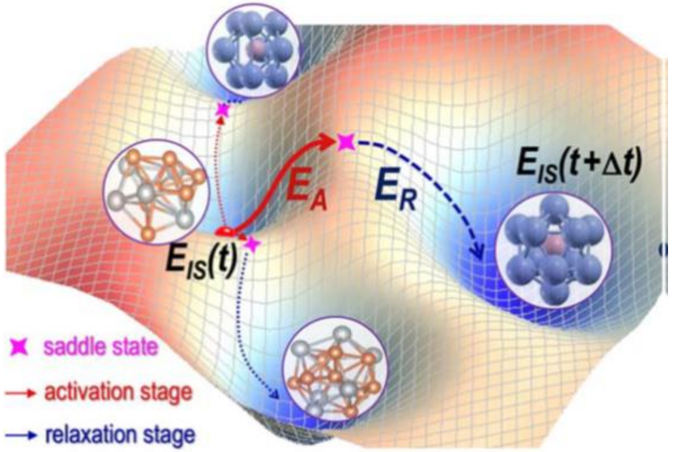
Alloy: Fe-25at%-X25at%Y at 800K

Pure Fe at 800K

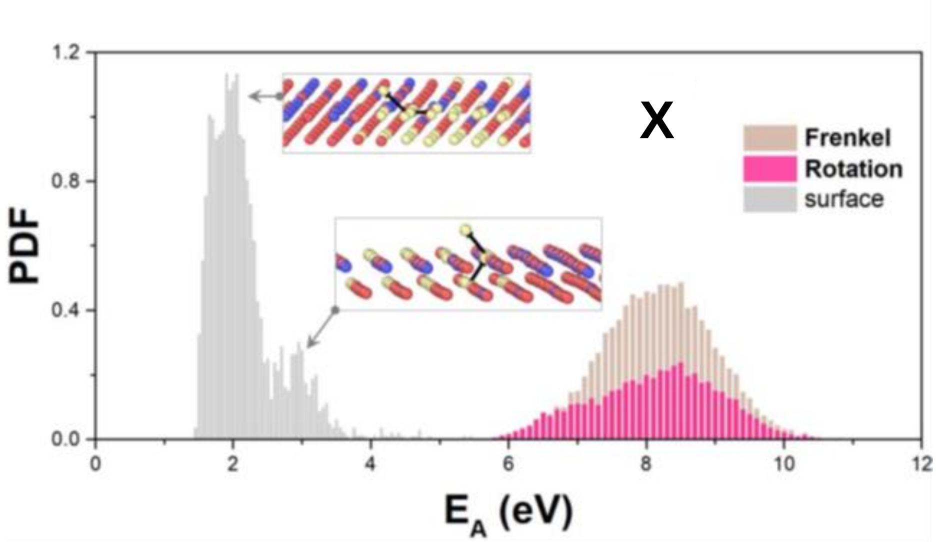
- Conclusion: alloy has advantage over pure Fe in terms of corrosion, especially when H_2O is dominant.

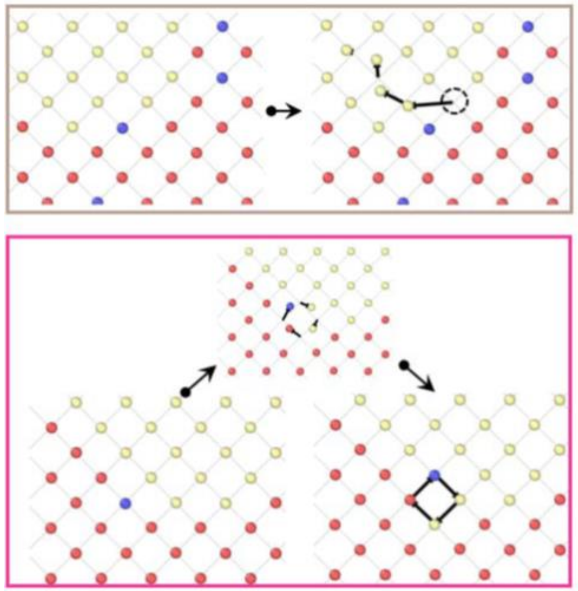
Technical Accomplishment

- PEL is utilized to understand the atomic migration mechanism w/o pre-assumption
  - The migration mechanisms and activation barrier spectrum are obtained bv activation relaxation technique (ART)



Step 0: Prepare the system (*i.e.* set up the initial state)
Step 1: Introduce location-specific random perturbations
Step 2: Let the system evolve under ART algorithm (through PEL curvature analysis)
Step 3: Identify the connecting saddle and final states without pre-assumptions





viable atomic rearrangement mechanisms and barriers can be obtained without invoking pre-assumptions.

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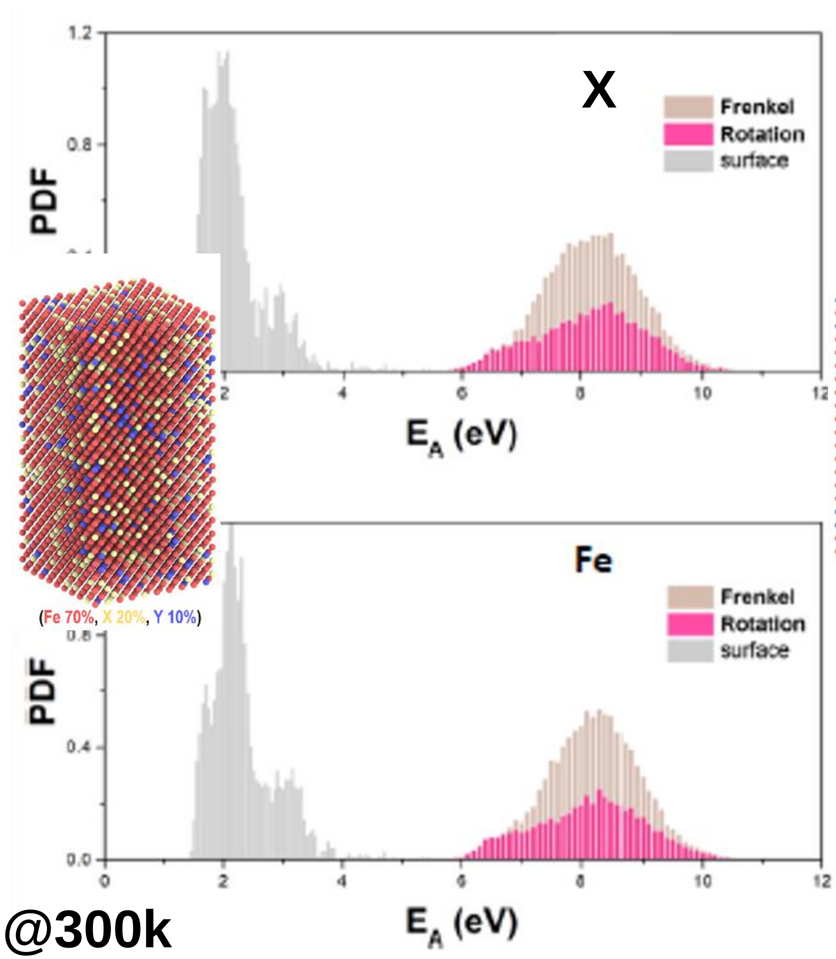
Technical Accomplishment

- Random solid solution vs segregated structure: Cr has higher mobility than Fe at surface in latter case



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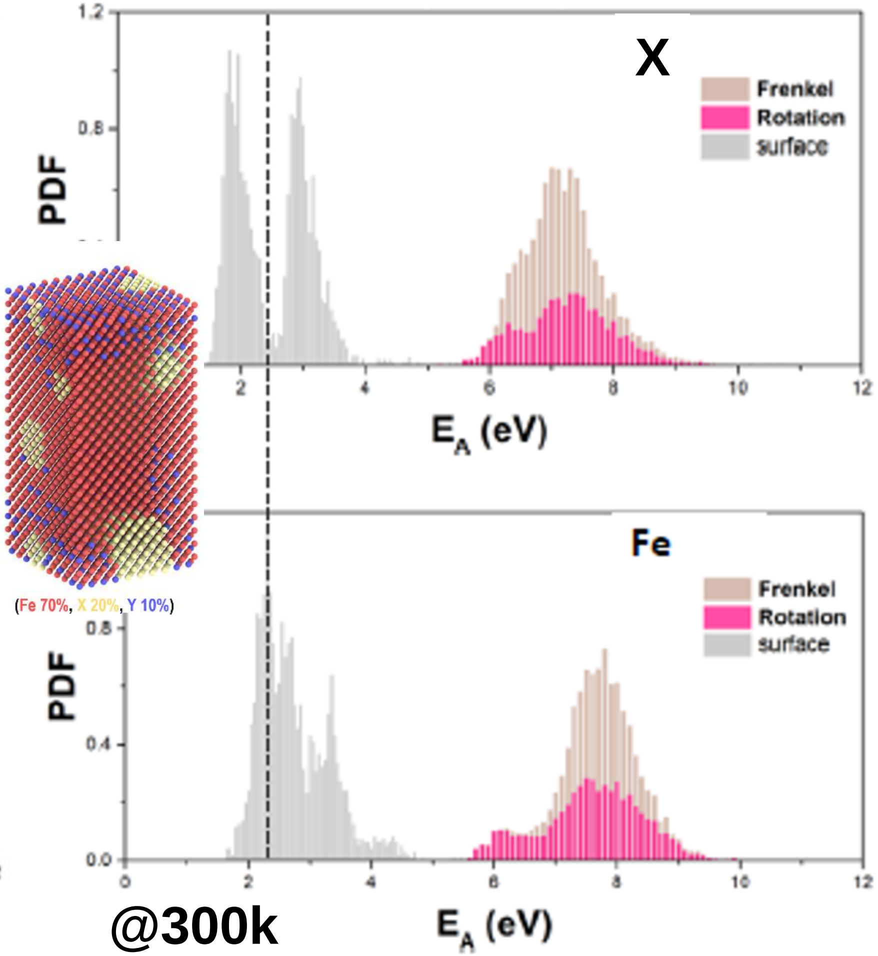

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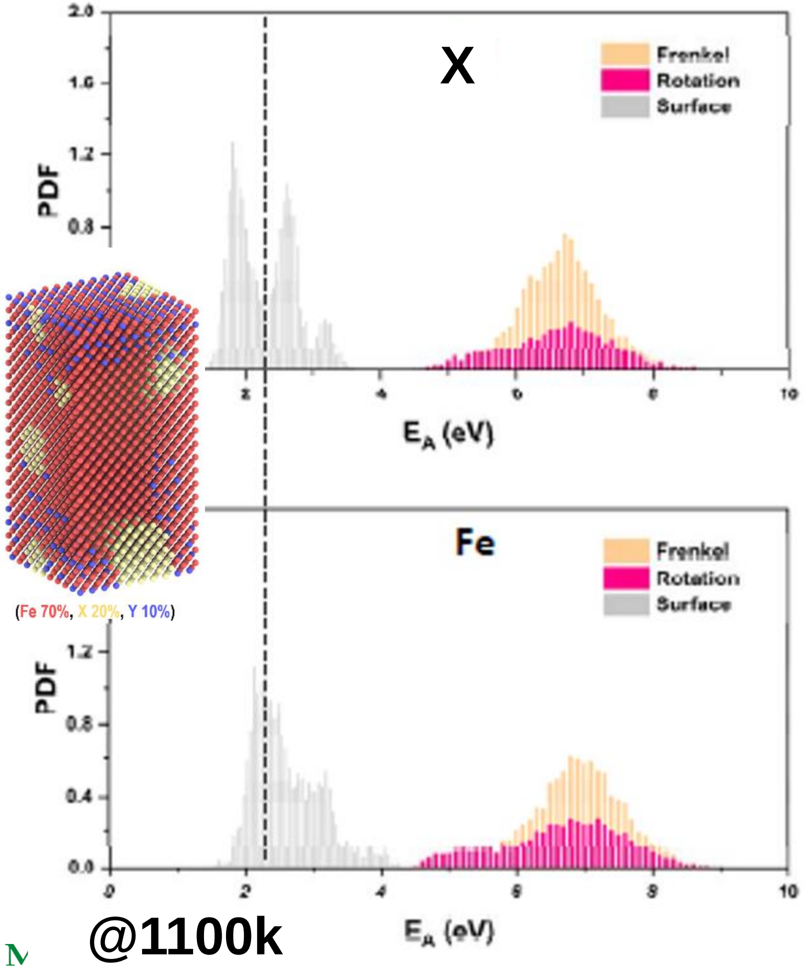
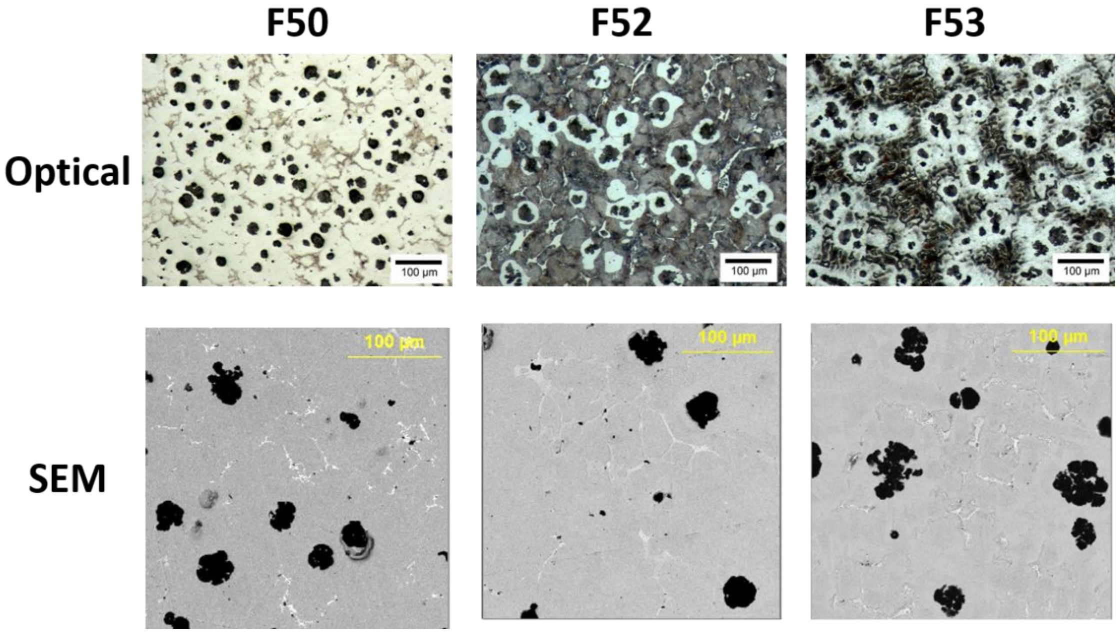
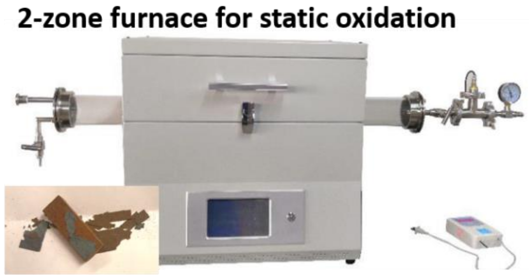


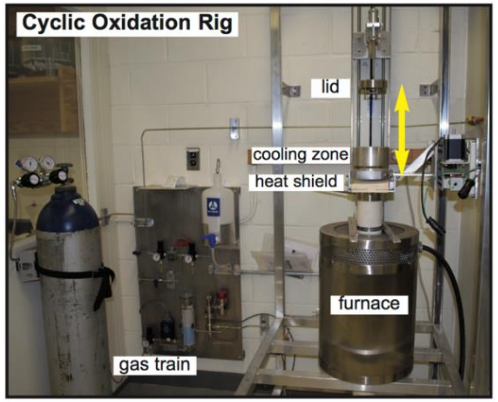
@1100k

Technical Accomplishment

- Four Sets of SiMo-type alloys were cast
  - F50: base SiMo-type cast iron, F51: F50 with 0.5wt% addition of *X*, F52: F50 with 1.0wt% addition of *X*, F52: F50 with 3wt% addition of *Y (X,Y are the alloying element studied by corrosion/oxidation performance modeling)*
- Static and cyclic corrosion/oxidation tests

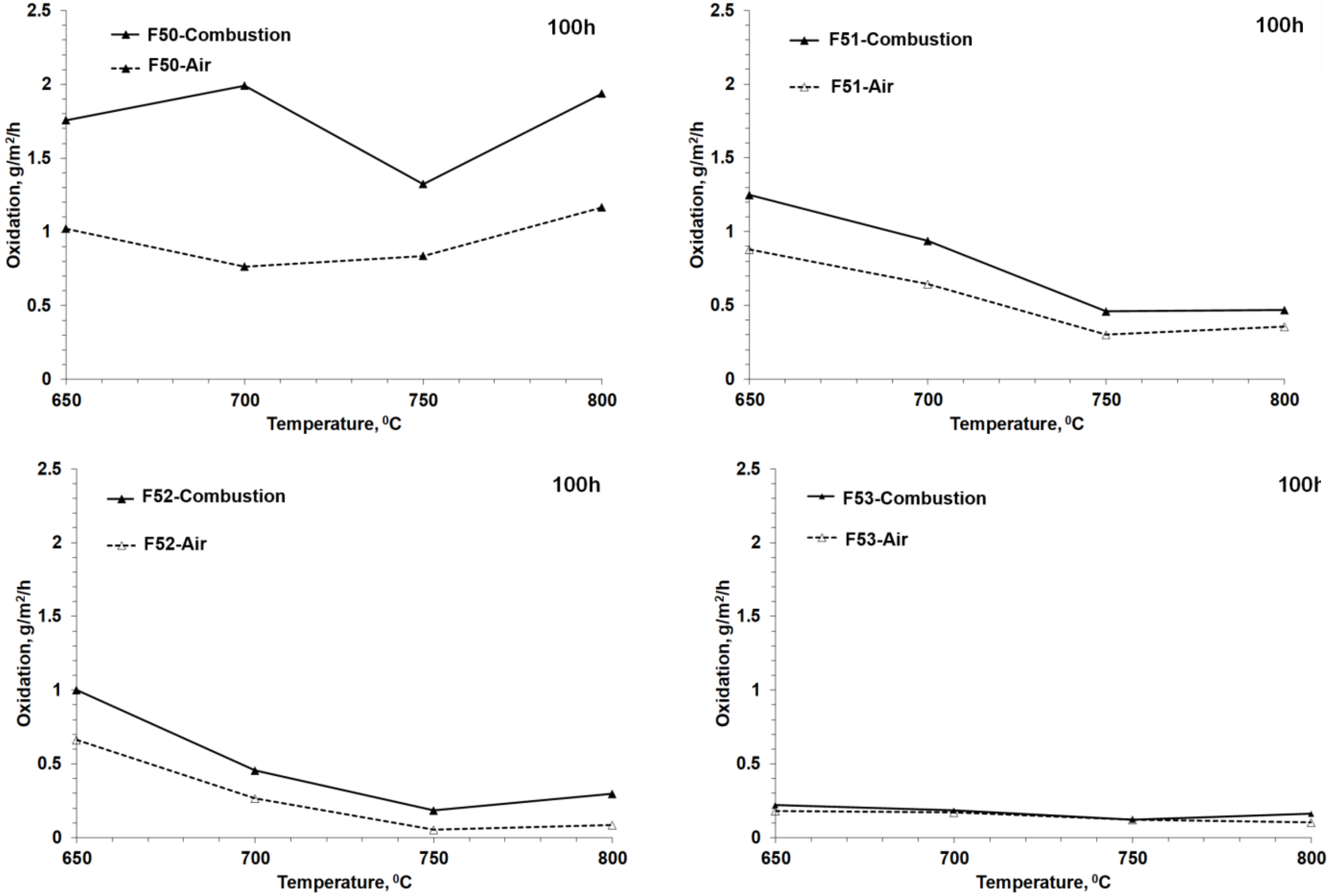


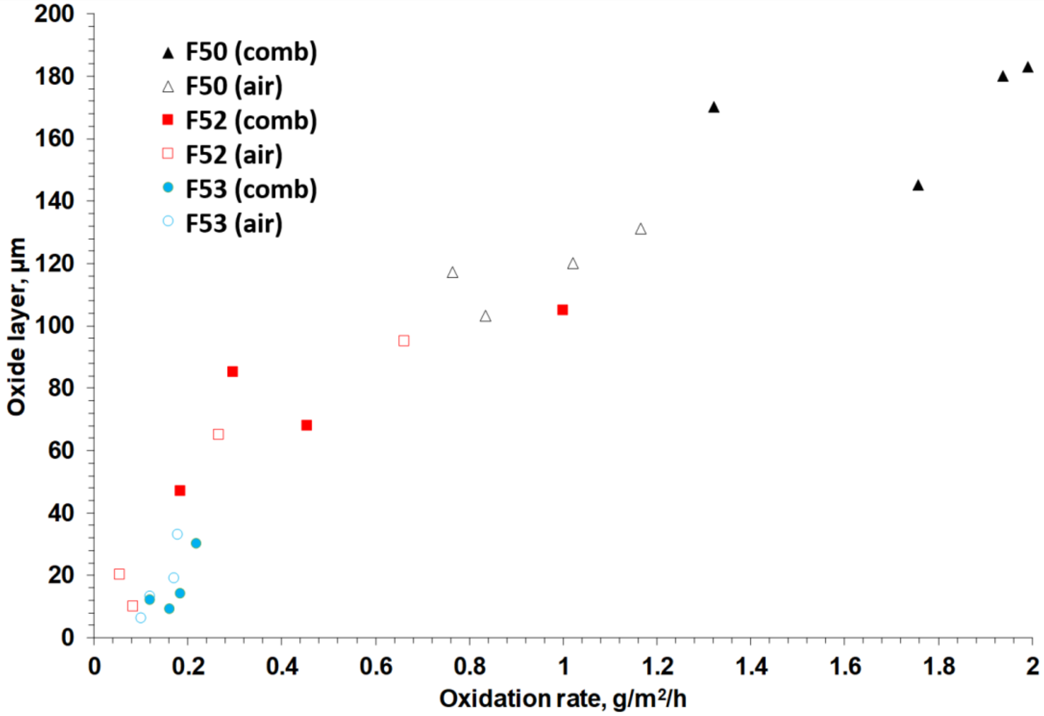




Technical Accomplishment

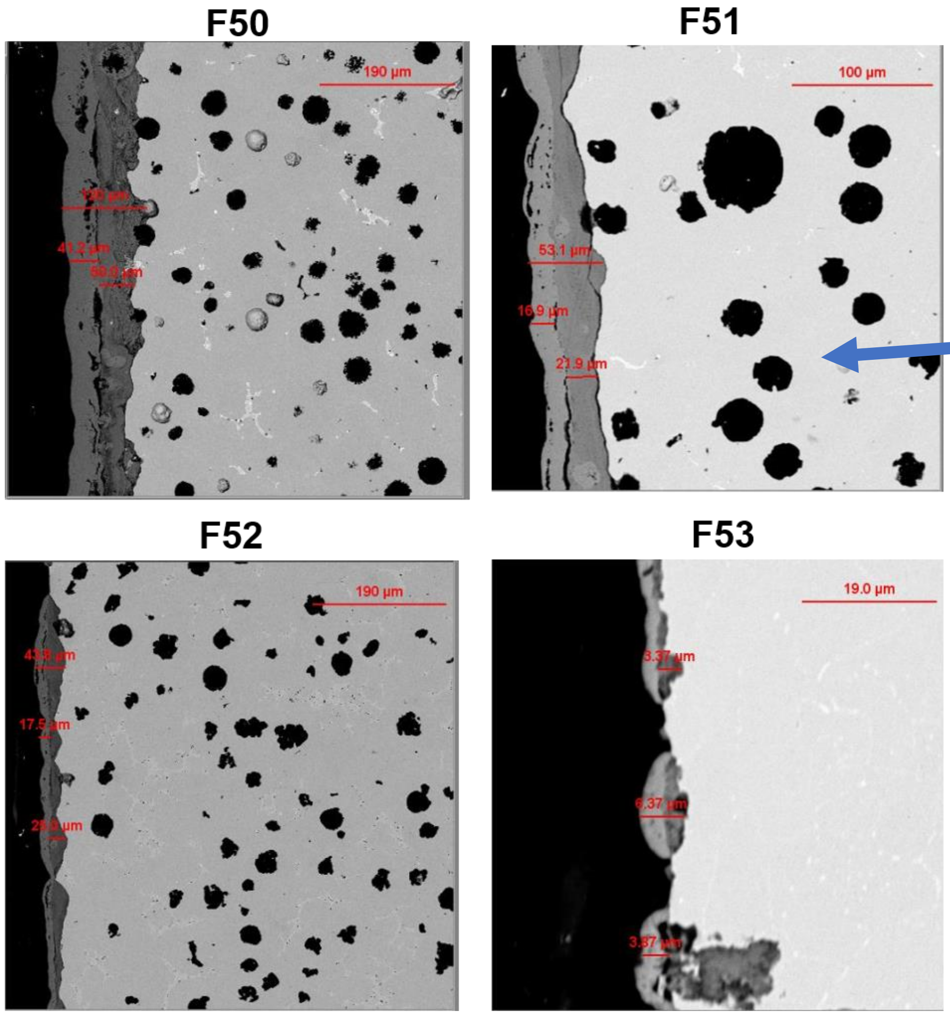
- Static oxidation is quantified by the total weight change subtracting the weigh loss due to de-carbonization
- Alloying elements improve oxidation performance

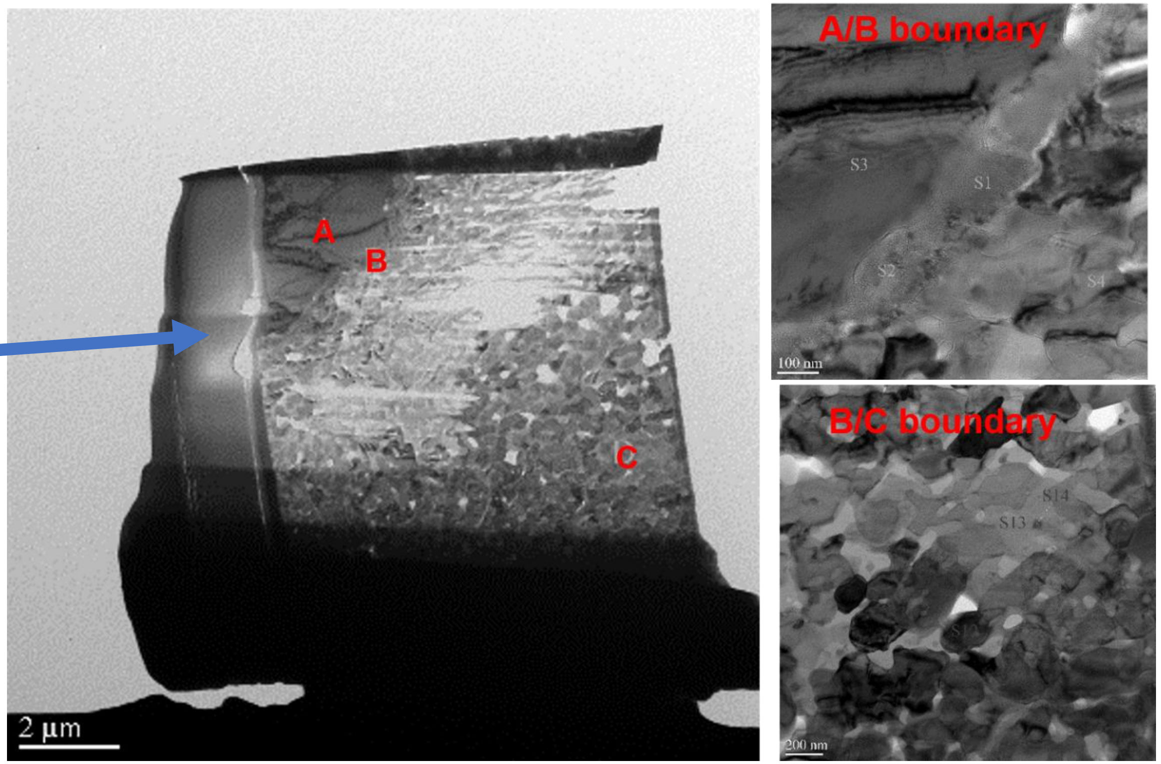




Technical Accomplishment

- SEM characterization of oxidation layers

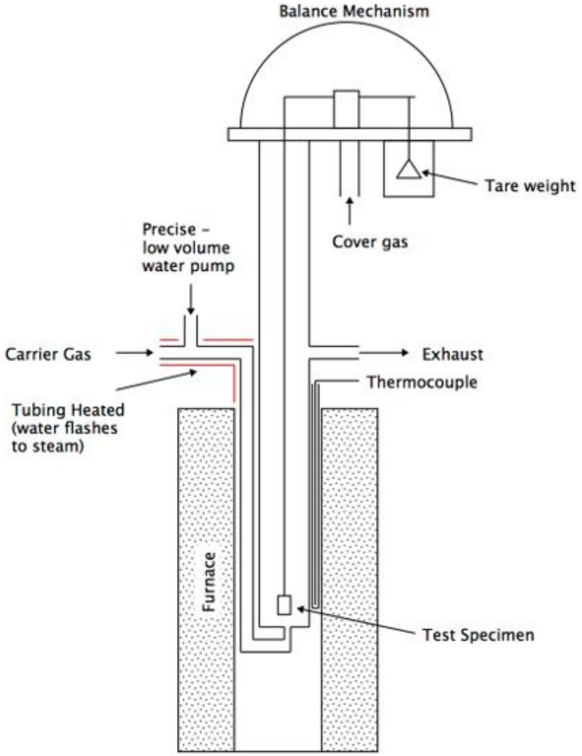


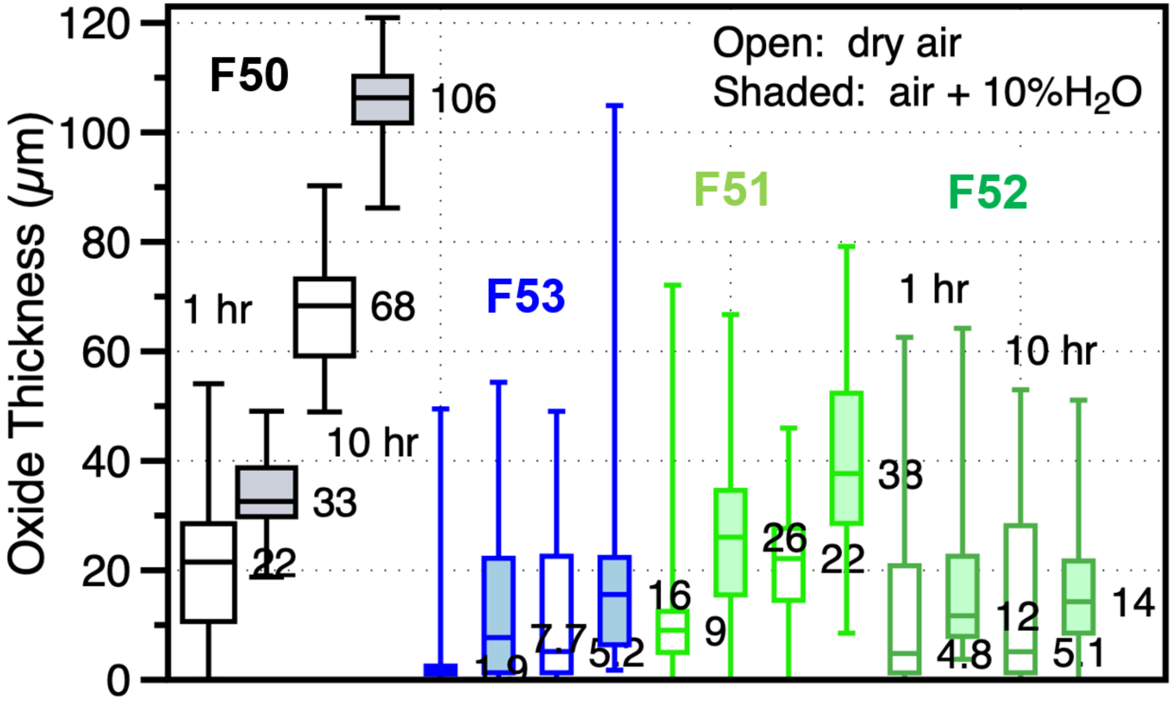


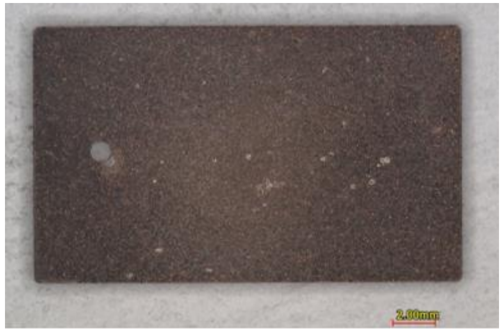
- TEM characterization of different oxidation layers fir F51 in air, 750C100hr
  - A-matrix
  - B-sublayer
  - C-internal layer

Technical Accomplishment

- Cyclic corrosion/oxidation test condition
  - Temperature 800K and 6min per cycle
  - Environment: dry air, air+10%H2O, and argon
- Alloying elements improve corrosion/oxidation performance

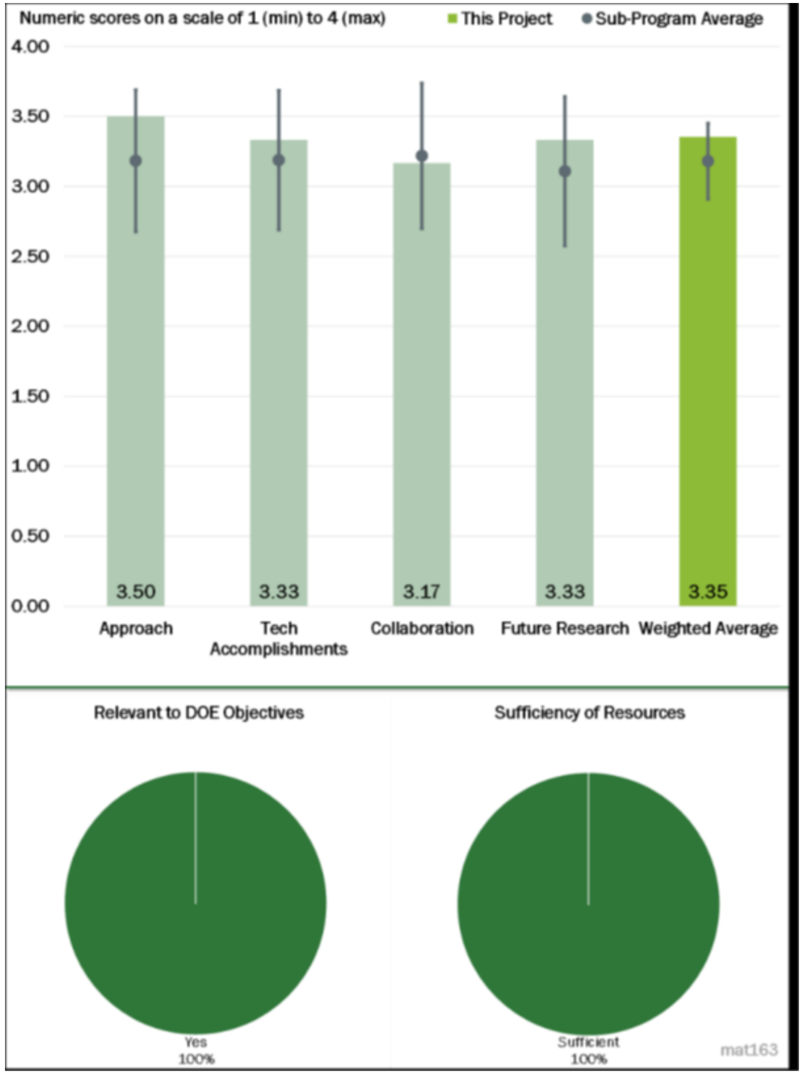






Responses to Previous Years Comments

- The reviewer stated that “The reviewer said the team did show some collaboration, but it was not clear on who was doing what during the presentation. It would be good to show a table explaining the team responsibility with the research.”
- Response: the works undertook by all the participants in this project will be elucidated in the following slides. In addition, to fill the gas between the micro-scale and meso-scale models, Professor Fan Yue from University of Michigan join this team and he will contribute his expertise on PEL modeling to develop a more reliable and comprehensive ICME work for corrosion/oxidation performance

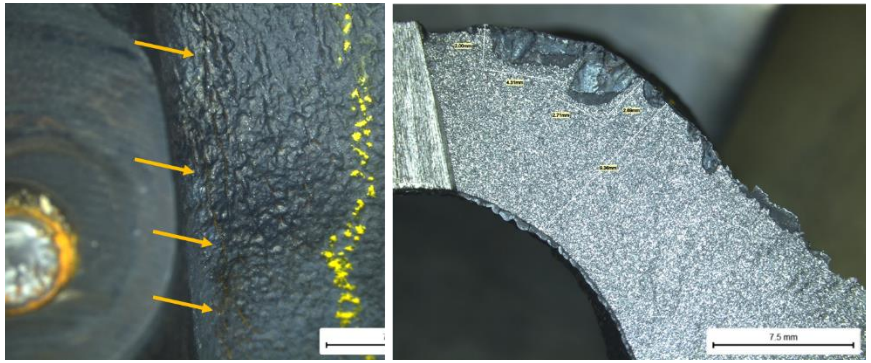


Collaboration

- Ford Motor Company (Mei Li):
  - TMF tests and empirical model development
  - Components demonstration
- The Ohio State University (Christophe Taylor):
  - DFT and ReaxFF MD simulation
- University of Michigan (Yue Fan):
  - PEL modeling simulation
- Missouri Science and Technology (Simon Lekakh):
  - Sample Preparation and static oxidation tests
- Oak Ridge National Laboratory (Bruce Pint):
  - Cyclic Oxidation tests

Remaining Challenges and Barriers

- Gaps between micro-scale and meso-scale models for corrosion/oxidation performance exists due to the large disparity in time and length scales;
- The simulation results of micro-scale modeling including DFT, ReaxFF MD, and PEL modeling, are hard to be validated by direct and quantitative experiments
- The TMF rigs for in-site corrosion/oxidation-fatigue test need to be designed and developed
- Components demonstration by dyno and vehicle tests



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Future Research

- More reliable force field for ReaxFF MD simulation is going to be developed by DFT calculation
- Grain boundary and other defects that are thought to facilitate atomic migration will be considered in PEL modeling
- The TEM and SEM characterizations of cyclic oxidized samples are on-going
- TMF tests for F50, F51, F52, and F53, including as-cast and as-oxidized, are on-going
- Upgrade of TMF rigs with chambers for in-site corrosion/oxidation-fatigue tests
- Any proposed future work is subject to change based on funding level

Summary

- ReaxFF MD simulation was developed to understand the chemical reaction between SiMo-type alloys with two different alloying elements and exhaust gas spieces;
- PEL modeling was used to study the atomic migration mechanism for SiMo-type alloys
- Static and cyclic corrosion/oxidation tests were complete and the oxidation are being quantified